Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2026 – 10:08 AM JST

PDB ID	:	22TG / pdb_000022tg
Title	:	Crystal Structure of MYST histone acetyltransferase KAT6A in complex with Compound 22
Authors	:	NarasimhaRao, K.; Vijayshankar, N.; SumalathaRani, T.; Kalishankar, B.; Chandregowda, V.; Chandrasekar, A.; Susanta, S.; Raymond, A.N.; David, C.M.
Deposited on	:	2026-01-22
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

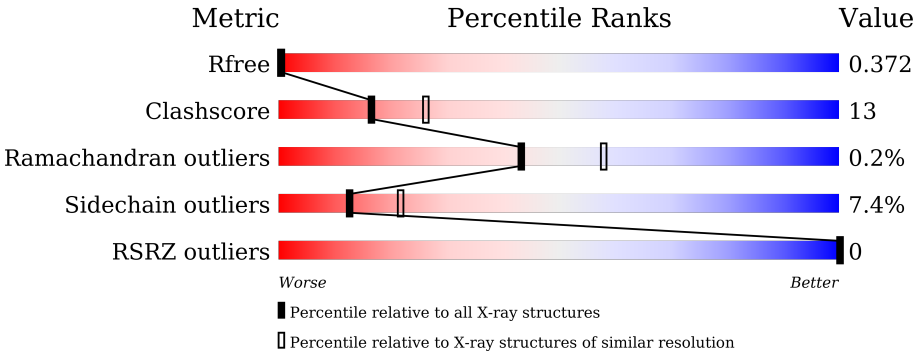
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	295	61% 24% •• 13%
1	C	295	59% 26% • 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4490 atoms, of which 40 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone acetyltransferase KAT8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2121	1384	342	383	12			
1	C	259	Total	C	N	O	S	0	0	0
			2144	1400	346	386	12			

There are 50 discrepancies between the modelled and reference sequences:

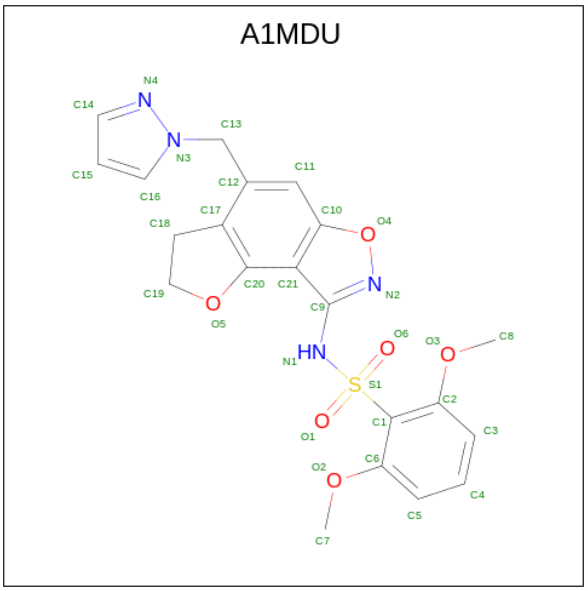
Chain	Residue	Modelled	Actual	Comment	Reference
A	485	MET	-	initiating methionine	UNP Q9H7Z6
A	486	GLY	-	expression tag	UNP Q9H7Z6
A	487	SER	-	expression tag	UNP Q9H7Z6
A	488	SER	-	expression tag	UNP Q9H7Z6
A	489	HIS	-	expression tag	UNP Q9H7Z6
A	490	HIS	-	expression tag	UNP Q9H7Z6
A	491	HIS	-	expression tag	UNP Q9H7Z6
A	492	HIS	-	expression tag	UNP Q9H7Z6
A	493	HIS	-	expression tag	UNP Q9H7Z6
A	494	HIS	-	expression tag	UNP Q9H7Z6
A	495	SER	-	expression tag	UNP Q9H7Z6
A	496	SER	-	expression tag	UNP Q9H7Z6
A	497	GLY	-	expression tag	UNP Q9H7Z6
A	498	LEU	-	expression tag	UNP Q9H7Z6
A	499	VAL	-	expression tag	UNP Q9H7Z6
A	500	PRO	-	expression tag	UNP Q9H7Z6
A	501	ARG	-	expression tag	UNP Q9H7Z6
A	502	GLY	-	expression tag	UNP Q9H7Z6
A	503	SER	-	expression tag	UNP Q9H7Z6
A	579	HIS	TYR	engineered mutation	UNP Q9H7Z6
A	645	SER	ALA	engineered mutation	UNP Q9H7Z6
A	648	MET	LEU	engineered mutation	UNP Q9H7Z6
A	649	ILE	THR	engineered mutation	UNP Q9H7Z6
A	660	ARG	LYS	engineered mutation	UNP Q9H7Z6
A	702	ASN	ILE	engineered mutation	UNP Q9H7Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	485	MET	-	initiating methionine	UNP Q9H7Z6
C	486	GLY	-	expression tag	UNP Q9H7Z6
C	487	SER	-	expression tag	UNP Q9H7Z6
C	488	SER	-	expression tag	UNP Q9H7Z6
C	489	HIS	-	expression tag	UNP Q9H7Z6
C	490	HIS	-	expression tag	UNP Q9H7Z6
C	491	HIS	-	expression tag	UNP Q9H7Z6
C	492	HIS	-	expression tag	UNP Q9H7Z6
C	493	HIS	-	expression tag	UNP Q9H7Z6
C	494	HIS	-	expression tag	UNP Q9H7Z6
C	495	SER	-	expression tag	UNP Q9H7Z6
C	496	SER	-	expression tag	UNP Q9H7Z6
C	497	GLY	-	expression tag	UNP Q9H7Z6
C	498	LEU	-	expression tag	UNP Q9H7Z6
C	499	VAL	-	expression tag	UNP Q9H7Z6
C	500	PRO	-	expression tag	UNP Q9H7Z6
C	501	ARG	-	expression tag	UNP Q9H7Z6
C	502	GLY	-	expression tag	UNP Q9H7Z6
C	503	SER	-	expression tag	UNP Q9H7Z6
C	579	HIS	TYR	engineered mutation	UNP Q9H7Z6
C	645	SER	ALA	engineered mutation	UNP Q9H7Z6
C	648	MET	LEU	engineered mutation	UNP Q9H7Z6
C	649	ILE	THR	engineered mutation	UNP Q9H7Z6
C	660	ARG	LYS	engineered mutation	UNP Q9H7Z6
C	702	ASN	ILE	engineered mutation	UNP Q9H7Z6

- Molecule 2 is 2,6-dimethoxy- {N}-[4-(pyrazol-1-ylmethyl)-2,3-dihydrofuro[2,3-e][1,2]benzoxazol-8-yl]benzenesulfonamide (CCD ID: A1MDU) (formula: $C_{21}H_{20}N_4O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			52	21	20	4	6	1		
2	C	1	Total	C	H	N	O	S	0	0
			52	21	20	4	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	C	52	Total	O	0	0
			52	52		

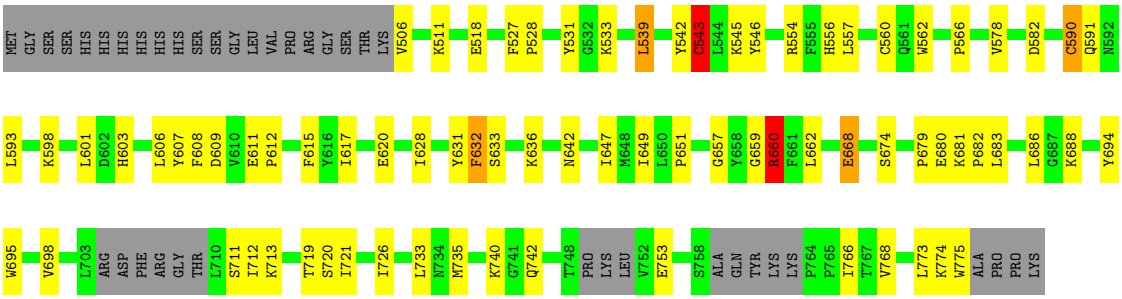
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Histone acetyltransferase KAT8

Chain A:

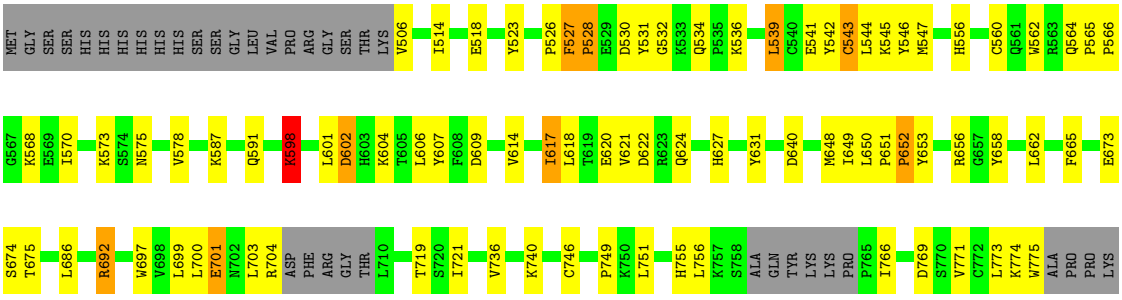




• Molecule 1: Histone acetyltransferase KAT8

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.69Å 46.41Å 120.92Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	43.32 – 2.40 43.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (43.32-2.40) 98.6 (43.32-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.293 , 0.372 0.293 , 0.372	Depositor DCC
R_{free} test set	1320 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 9.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.357 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4490	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1MDU, ALY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.58	0/2168	1.21	8/2932 (0.3%)
1	C	0.55	0/2192	1.20	4/2965 (0.1%)
All	All	0.56	0/4360	1.20	12/5897 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	590	CYS	CB-CA-C	7.21	122.75	110.79
1	A	651	PRO	N-CA-C	6.60	118.75	110.70
1	A	542	TYR	CA-C-N	6.33	128.76	120.28
1	A	542	TYR	C-N-CA	6.33	128.76	120.28
1	A	620	GLU	CB-CA-C	-6.24	100.08	110.19
1	C	527	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	632	PHE	CA-CB-CG	6.10	119.90	113.80
1	A	543	CYS	N-CA-C	-6.07	104.66	111.28
1	C	598	LYS	CB-CA-C	5.83	122.99	110.21
1	C	528	PRO	CA-C-N	5.55	127.99	120.38
1	C	528	PRO	C-N-CA	5.55	127.99	120.38
1	A	774	LYS	CB-CA-C	-5.14	103.93	111.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	554	ARG	Sidechain
1	A	660	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2121	0	2087	53	1
1	C	2144	0	2116	56	1
2	A	32	20	0	2	0
2	C	32	20	0	0	0
3	A	69	0	0	4	0
3	C	52	0	0	10	0
All	All	4450	40	4203	109	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:CYS:SG	1:A:556:HIS:NE2	2.29	1.03
1:C:736:VAL:HG12	3:C:914:HOH:O	1.72	0.89
1:A:647:ILE:HD11	1:A:662:LEU:HB3	1.53	0.89
1:C:541:GLU:OE1	1:C:627:HIS:HD2	1.57	0.88
1:C:746:CYS:HB3	3:C:911:HOH:O	1.75	0.86
1:A:660:ARG:HH21	1:A:660:ARG:CG	1.90	0.85
1:A:606:LEU:HD21	1:A:609:ASP:O	1.82	0.79
1:A:753:GLU:HA	1:A:753:GLU:OE1	1.84	0.77
1:C:598:LYS:HE2	1:C:601:LEU:O	1.85	0.75
1:C:618:LEU:HB2	1:C:662:LEU:HD21	1.70	0.73
1:A:775:TRP:CD1	1:A:775:TRP:C	2.68	0.72
1:C:648:MET:C	1:C:649:ILE:HD13	2.14	0.71
1:C:648:MET:O	1:C:649:ILE:HD13	1.92	0.70
1:A:660:ARG:NH2	1:A:660:ARG:HG3	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:LYS:HB3	3:C:922:HOH:O	1.90	0.69
1:A:660:ARG:CG	1:A:660:ARG:NH2	2.52	0.69
1:A:649:ILE:HD11	1:A:662:LEU:HD12	1.77	0.66
1:A:593:LEU:HD23	1:A:615:PHE:CD2	2.30	0.66
1:C:562:TRP:HZ3	1:C:566:PRO:HD3	1.60	0.66
1:C:539:LEU:HD22	1:C:546:TYR:HA	1.78	0.66
1:A:668:GLU:HG2	1:A:768:VAL:HG11	1.77	0.65
1:A:660:ARG:HH21	1:A:660:ARG:HG2	1.62	0.64
1:C:602:ASP:OD1	1:C:602:ASP:N	2.24	0.64
1:A:775:TRP:C	1:A:775:TRP:HD1	2.06	0.63
1:C:578:VAL:HG11	1:C:665:PHE:CE2	2.34	0.63
1:A:560:CYS:HB3	3:A:939:HOH:O	1.98	0.62
1:A:660:ARG:HH21	1:A:660:ARG:HG3	1.60	0.61
1:A:775:TRP:CD1	1:A:775:TRP:O	2.54	0.61
1:C:692:ARG:HH11	1:C:692:ARG:HG3	1.67	0.59
1:C:622:ASP:OD1	1:C:624:GLN:HB2	2.03	0.59
1:A:598:LYS:HD3	1:A:607:TYR:HE1	1.67	0.58
1:C:541:GLU:OE1	1:C:627:HIS:CD2	2.48	0.58
1:C:518:GLU:OE2	1:C:536:LYS:NZ	2.38	0.57
1:A:593:LEU:CD2	1:A:615:PHE:CD2	2.87	0.57
1:C:536:LYS:CB	3:C:922:HOH:O	2.51	0.57
1:A:659:GLY:HA3	2:A:801:A1MDU:N1	2.20	0.56
1:A:688:LYS:HE2	3:A:919:HOH:O	2.04	0.56
1:A:647:ILE:CD1	1:A:662:LEU:HB3	2.31	0.56
1:A:545:LYS:HD3	1:A:556:HIS:CE1	2.41	0.56
1:C:699:LEU:O	1:C:703:LEU:HG	2.05	0.56
1:A:649:ILE:CD1	1:A:662:LEU:HD12	2.38	0.54
1:C:587:LYS:O	1:C:591:GLN:HG3	2.08	0.54
1:A:611:GLU:N	1:A:612:PRO:CD	2.71	0.53
1:C:620:GLU:OE2	1:C:658:TYR:OH	2.14	0.53
1:C:545:LYS:HA	3:C:903:HOH:O	2.07	0.53
1:C:556:HIS:CD2	1:C:560:CYS:HB2	2.43	0.52
1:C:703:LEU:O	1:C:704:ARG:C	2.52	0.52
1:A:647:ILE:HD11	1:A:662:LEU:CB	2.31	0.52
1:C:578:VAL:HA	1:C:617:ILE:O	2.09	0.52
1:C:526:PRO:HG3	1:C:607:TYR:CE2	2.45	0.52
1:C:740:LYS:CE	3:C:941:HOH:O	2.57	0.52
1:C:703:LEU:O	1:C:704:ARG:O	2.28	0.52
1:A:719:THR:O	1:A:720:SER:HB2	2.09	0.51
1:A:657:GLY:N	2:A:801:A1MDU:O1	2.36	0.50
1:A:721:ILE:HG22	1:A:726:ILE:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:PRO:O	1:C:653:TYR:N	2.45	0.50
1:C:704:ARG:C	3:C:929:HOH:O	2.55	0.49
1:C:598:LYS:HD2	1:C:604:ALY:O	2.12	0.49
1:A:562:TRP:CZ3	1:A:566:PRO:HD3	2.48	0.49
1:A:582:ASP:OD1	1:A:636:LYS:NZ	2.39	0.49
1:C:653:TYR:O	1:C:656:ARG:HB2	2.12	0.49
1:A:562:TRP:HZ3	1:A:566:PRO:HD3	1.79	0.48
1:C:652:PRO:O	1:C:656:ARG:CZ	2.62	0.47
1:A:679:PRO:HB2	1:A:683:LEU:HD21	1.97	0.47
1:A:527:PHE:O	1:A:528:PRO:C	2.58	0.47
1:A:539:LEU:HD22	1:A:546:TYR:HB3	1.97	0.46
1:A:733:LEU:HB3	1:A:735:MET:HE3	1.97	0.46
1:C:562:TRP:CZ3	1:C:566:PRO:HD3	2.46	0.46
1:A:694:TYR:CZ	1:A:698:VAL:HG21	2.50	0.46
1:C:564:GLN:HG3	1:C:565:PRO:O	2.16	0.46
1:C:749:PRO:HB3	3:C:929:HOH:O	2.15	0.46
1:C:523:TYR:CE1	1:C:602:ASP:HB3	2.51	0.46
1:A:711:SER:C	1:A:713:LYS:N	2.72	0.46
1:A:511:LYS:HE3	1:A:518:GLU:HB3	1.99	0.45
1:A:528:PRO:HB2	1:A:531:TYR:HD1	1.80	0.45
1:A:590:CYS:O	1:A:593:LEU:HB3	2.16	0.45
1:C:532:GLY:C	1:C:534:GLN:H	2.24	0.45
1:A:632:PHE:HB3	1:A:647:ILE:HD12	1.99	0.45
1:C:700:LEU:HB3	1:C:756:LEU:HD21	1.97	0.45
1:A:533:LYS:HG3	3:A:923:HOH:O	2.17	0.44
1:C:606:LEU:C	1:C:606:LEU:HD23	2.41	0.44
1:C:604:ALY:HE3	1:C:631:TYR:OH	2.17	0.44
1:A:628:ILE:O	1:A:628:ILE:HG23	2.17	0.44
1:A:631:TYR:HE2	1:A:633:SER:HB3	1.82	0.44
1:A:611:GLU:N	1:A:612:PRO:HD3	2.33	0.43
3:A:957:HOH:O	1:C:774:LYS:HE2	2.18	0.43
1:A:578:VAL:HA	1:A:617:ILE:O	2.18	0.43
1:A:668:GLU:HG2	1:A:768:VAL:CG1	2.48	0.43
1:C:575:ASN:O	1:C:621:VAL:HG23	2.18	0.43
1:A:601:LEU:HA	1:A:601:LEU:HD23	1.82	0.43
1:C:650:LEU:O	1:C:651:PRO:C	2.62	0.43
1:C:697:TRP:C	1:C:697:TRP:CD1	2.96	0.43
1:C:697:TRP:NE1	1:C:701:GLU:OE1	2.52	0.43
1:A:695:TRP:CD1	1:A:721:ILE:HD13	2.54	0.42
1:C:539:LEU:HD23	1:C:539:LEU:N	2.34	0.42
1:C:673:GLU:HB3	1:C:675:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:LYS:NZ	1:C:570:ILE:HG22	2.34	0.42
1:C:573:LYS:HE3	1:C:769:ASP:OD2	2.19	0.42
1:A:603:HIS:ND1	1:A:682:PRO:HG2	2.35	0.42
1:A:711:SER:O	1:A:712:ILE:C	2.63	0.42
1:A:591:GLN:HG2	1:A:608:PHE:HA	2.02	0.41
1:C:543:CYS:O	1:C:544:LEU:HB2	2.20	0.41
1:C:740:LYS:HE2	3:C:941:HOH:O	2.19	0.41
1:C:651:PRO:C	1:C:653:TYR:H	2.27	0.41
1:C:719:THR:C	1:C:721:ILE:H	2.29	0.41
1:C:527:PHE:O	1:C:528:PRO:C	2.63	0.40
1:C:624:GLN:HG2	3:C:936:HOH:O	2.21	0.40
1:A:642:ASN:OD1	1:A:680:GLU:HG3	2.21	0.40
1:C:531:TYR:CE2	1:C:546:TYR:HD1	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:LYS:O	1:C:658:TYR:OH[1_565]	1.76	0.44

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	247/295 (84%)	233 (94%)	14 (6%)	0	100 100
1	C	252/295 (85%)	236 (94%)	15 (6%)	1 (0%)	30 43
All	All	499/590 (85%)	469 (94%)	29 (6%)	1 (0%)	43 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	652	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	237/271 (88%)	225 (95%)	12 (5%)	21 37
1	C	239/271 (88%)	216 (90%)	23 (10%)	8 12
All	All	476/542 (88%)	441 (93%)	35 (7%)	13 22

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	506	VAL
1	A	539	LEU
1	A	543	CYS
1	A	557	LEU
1	A	660	ARG
1	A	668	GLU
1	A	674	SER
1	A	681	LYS
1	A	686	LEU
1	A	742	GLN
1	A	766	ILE
1	A	773	LEU
1	C	506	VAL
1	C	514	ILE
1	C	530	ASP
1	C	539	LEU
1	C	542	TYR
1	C	543	CYS
1	C	547	MET
1	C	598	LYS
1	C	602	ASP
1	C	609	ASP
1	C	614	VAL

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Mol	Chain	Res	Type
1	C	617	ILE
1	C	640	ASP
1	C	674	SER
1	C	686	LEU
1	C	692	ARG
1	C	701	GLU
1	C	751	LEU
1	C	755	HIS
1	C	766	ILE
1	C	771	VAL
1	C	773	LEU
1	C	775	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	564	GLN
1	A	586	HIS
1	A	642	ASN
1	A	731	GLN
1	A	743	HIS
1	C	591	GLN
1	C	627	HIS
1	C	643	ASN
1	C	743	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	ALY	C	604	1	10,11,12	0.41	0	7,12,14	0.57	0
1	ALY	A	604	1	10,11,12	0.40	0	7,12,14	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	C	604	1	-	3/9/10/12	-
1	ALY	A	604	1	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	604	ALY	CG-CD-CE-NZ
1	C	604	ALY	CA-CB-CG-CD
1	A	604	ALY	CE-CD-CG-CB
1	C	604	ALY	CE-CD-CG-CB
1	A	604	ALY	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	604	ALY	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	A1MDU	C	801	-	36,36,36	2.51	9 (25%)	43,53,53	3.04	18 (41%)
2	A1MDU	A	801	-	36,36,36	2.71	8 (22%)	43,53,53	3.07	19 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1MDU	C	801	-	-	7/19/25/25	0/5/5/5
2	A1MDU	A	801	-	-	5/19/25/25	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1MDU	C9-N2	11.58	1.36	1.29
2	C	801	A1MDU	C9-N2	9.83	1.35	1.29
2	C	801	A1MDU	O4-N2	-5.48	1.37	1.43
2	A	801	A1MDU	O4-C10	-5.15	1.31	1.36
2	A	801	A1MDU	O4-N2	-4.83	1.38	1.43
2	A	801	A1MDU	O6-S1	4.81	1.49	1.43
2	C	801	A1MDU	O4-C10	-4.63	1.32	1.36
2	A	801	A1MDU	O1-S1	4.18	1.48	1.43
2	C	801	A1MDU	O6-S1	4.11	1.48	1.43
2	C	801	A1MDU	C2-C1	-3.75	1.38	1.41
2	C	801	A1MDU	O1-S1	3.67	1.47	1.43
2	A	801	A1MDU	N3-N4	2.87	1.41	1.36
2	A	801	A1MDU	C1-S1	2.85	1.83	1.79
2	C	801	A1MDU	C9-N1	-2.55	1.34	1.39
2	C	801	A1MDU	N3-N4	2.29	1.40	1.36
2	A	801	A1MDU	C21-C20	-2.18	1.35	1.40
2	C	801	A1MDU	C21-C20	-2.12	1.35	1.40

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	A1MDU	O6-S1-C1	-10.28	93.47	108.74
2	C	801	A1MDU	C1-S1-N1	9.90	120.34	106.76
2	C	801	A1MDU	C10-O4-N2	8.27	111.43	107.48
2	A	801	A1MDU	C10-O4-N2	7.44	111.04	107.48
2	C	801	A1MDU	C12-C13-N3	5.93	120.43	112.24
2	C	801	A1MDU	C20-C21-C9	5.83	138.35	132.39
2	C	801	A1MDU	O6-S1-O1	-5.43	112.87	119.55
2	A	801	A1MDU	O3-C2-C3	-5.23	115.41	124.37
2	A	801	A1MDU	C8-O3-C2	5.05	125.15	117.53
2	A	801	A1MDU	C1-S1-N1	4.98	113.59	106.76
2	A	801	A1MDU	N1-C9-N2	4.75	127.56	118.62
2	A	801	A1MDU	C20-C21-C9	4.28	136.76	132.39
2	C	801	A1MDU	O6-S1-C1	-4.13	102.60	108.74
2	C	801	A1MDU	N1-C9-N2	3.72	125.62	118.62
2	C	801	A1MDU	C6-C1-S1	-3.59	114.85	120.39
2	A	801	A1MDU	O2-C6-C5	-3.57	118.26	124.37
2	A	801	A1MDU	C2-C1-S1	3.47	125.75	120.39
2	A	801	A1MDU	C13-C12-C11	3.38	126.40	120.38
2	A	801	A1MDU	C12-C13-N3	3.36	116.87	112.24
2	C	801	A1MDU	C8-O3-C2	2.95	121.99	117.53
2	C	801	A1MDU	C7-O2-C6	2.87	121.86	117.53
2	A	801	A1MDU	C6-C1-S1	-2.84	116.00	120.39
2	C	801	A1MDU	C13-C12-C17	-2.78	115.97	121.50
2	C	801	A1MDU	O3-C2-C3	-2.69	119.77	124.37
2	A	801	A1MDU	C13-C12-C17	-2.68	116.16	121.50
2	C	801	A1MDU	C13-C12-C11	2.65	125.11	120.38
2	C	801	A1MDU	C19-O5-C20	2.62	108.91	107.04
2	A	801	A1MDU	C3-C2-C1	2.55	122.44	119.04
2	A	801	A1MDU	C13-N3-C16	2.50	131.59	127.85
2	A	801	A1MDU	C7-O2-C6	2.44	121.22	117.53
2	A	801	A1MDU	C10-C11-C12	-2.40	117.25	121.09
2	C	801	A1MDU	C10-C11-C12	-2.38	117.28	121.09
2	A	801	A1MDU	C13-N3-N4	-2.30	116.83	121.02
2	C	801	A1MDU	C2-C1-S1	2.28	123.92	120.39
2	C	801	A1MDU	O4-N2-C9	-2.24	102.55	104.15
2	C	801	A1MDU	C13-N3-N4	-2.08	117.23	121.02
2	A	801	A1MDU	O4-C10-C11	2.02	127.23	125.78

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	A1MDU	C6-C1-S1-N1

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Mol	Chain	Res	Type	Atoms
2	A	801	A1MDU	C2-C1-S1-N1
2	C	801	A1MDU	C6-C1-S1-N1
2	C	801	A1MDU	C2-C1-S1-N1
2	C	801	A1MDU	C1-C2-O3-C8
2	C	801	A1MDU	C3-C2-O3-C8
2	A	801	A1MDU	C6-C1-S1-O6
2	C	801	A1MDU	C6-C1-S1-O6
2	A	801	A1MDU	N2-C9-N1-S1
2	C	801	A1MDU	N2-C9-N1-S1
2	A	801	A1MDU	C12-C13-N3-C16
2	C	801	A1MDU	C12-C13-N3-C16

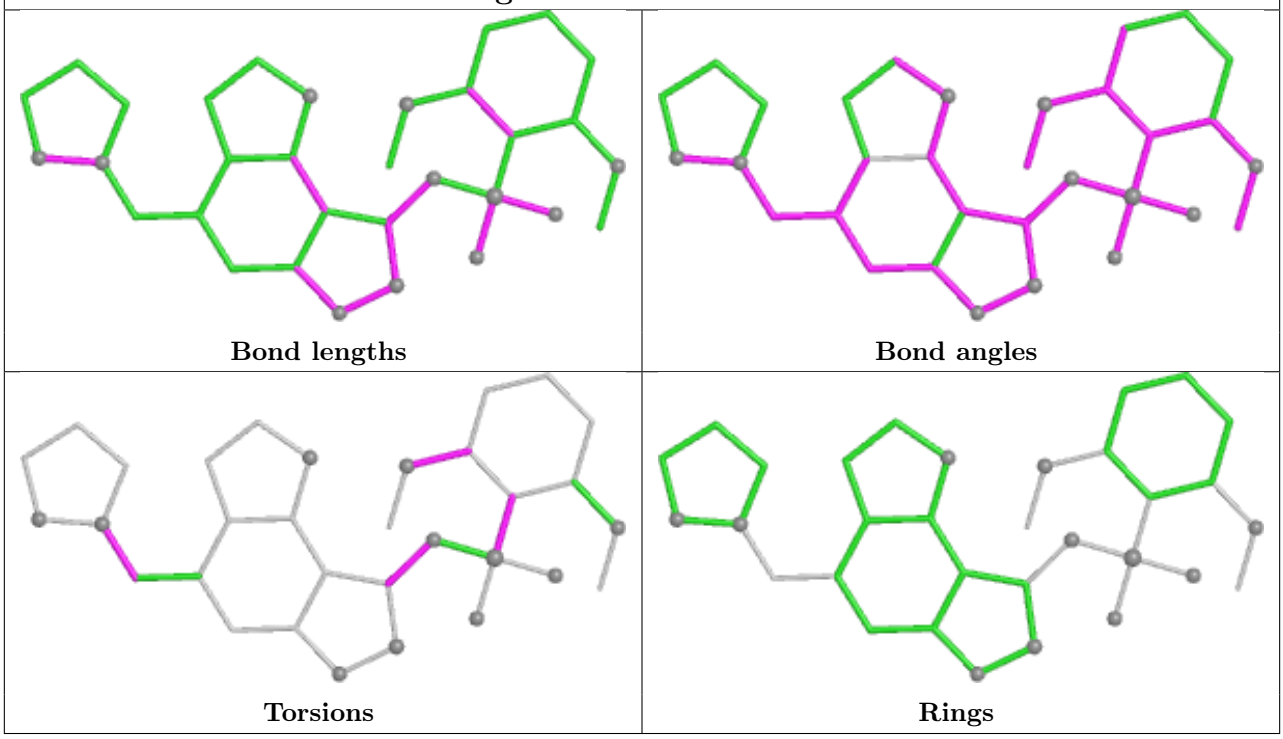
There are no ring outliers.

1 monomer is involved in 2 short contacts:

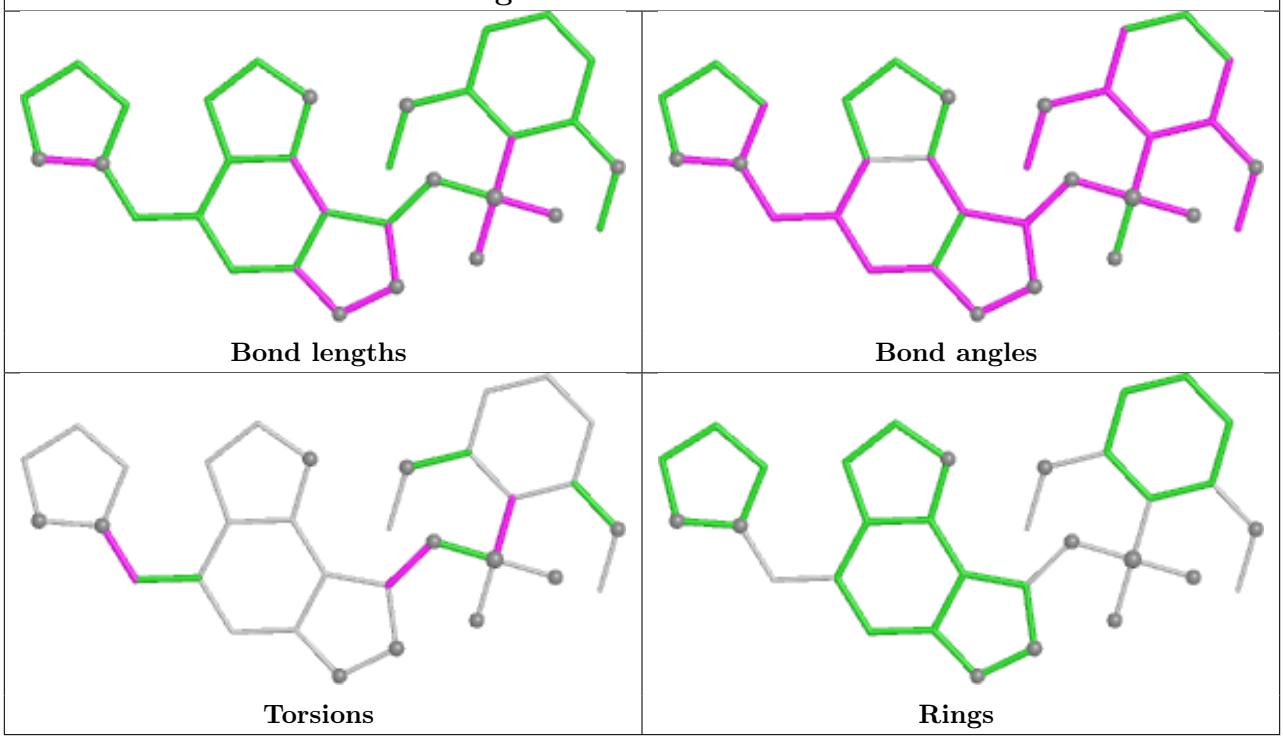
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	A1MDU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1MDU C 801



Ligand A1MDU A 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	255/295 (86%)	-0.80	0	100	100	16, 29, 53, 85	0
1	C	258/295 (87%)	-0.71	0	100	100	14, 30, 57, 72	0
All	All	513/590 (86%)	-0.75	0	100	100	14, 30, 55, 85	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	ALY	A	604	12/13	0.97	0.08	32,40,58,72	0
1	ALY	C	604	12/13	0.98	0.08	33,37,60,63	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

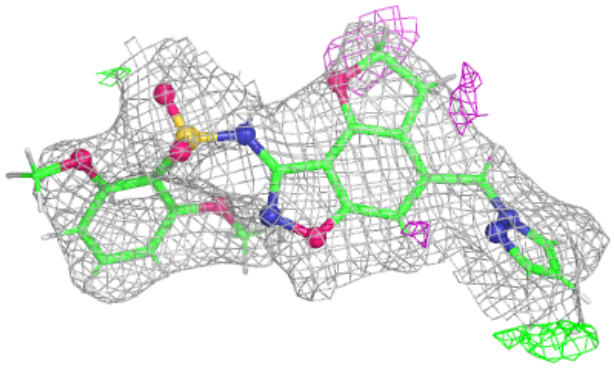
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

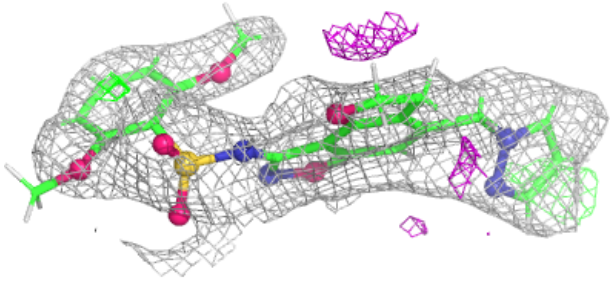
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1MDU	A	801	32/32	0.98	0.06	35,40,48,54	0
2	A1MDU	C	801	32/32	0.98	0.05	29,34,40,48	0

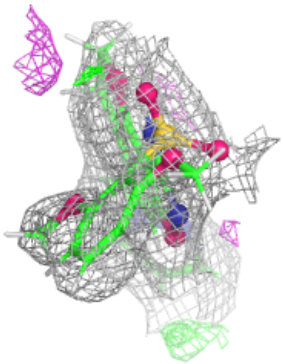
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1MDU A 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

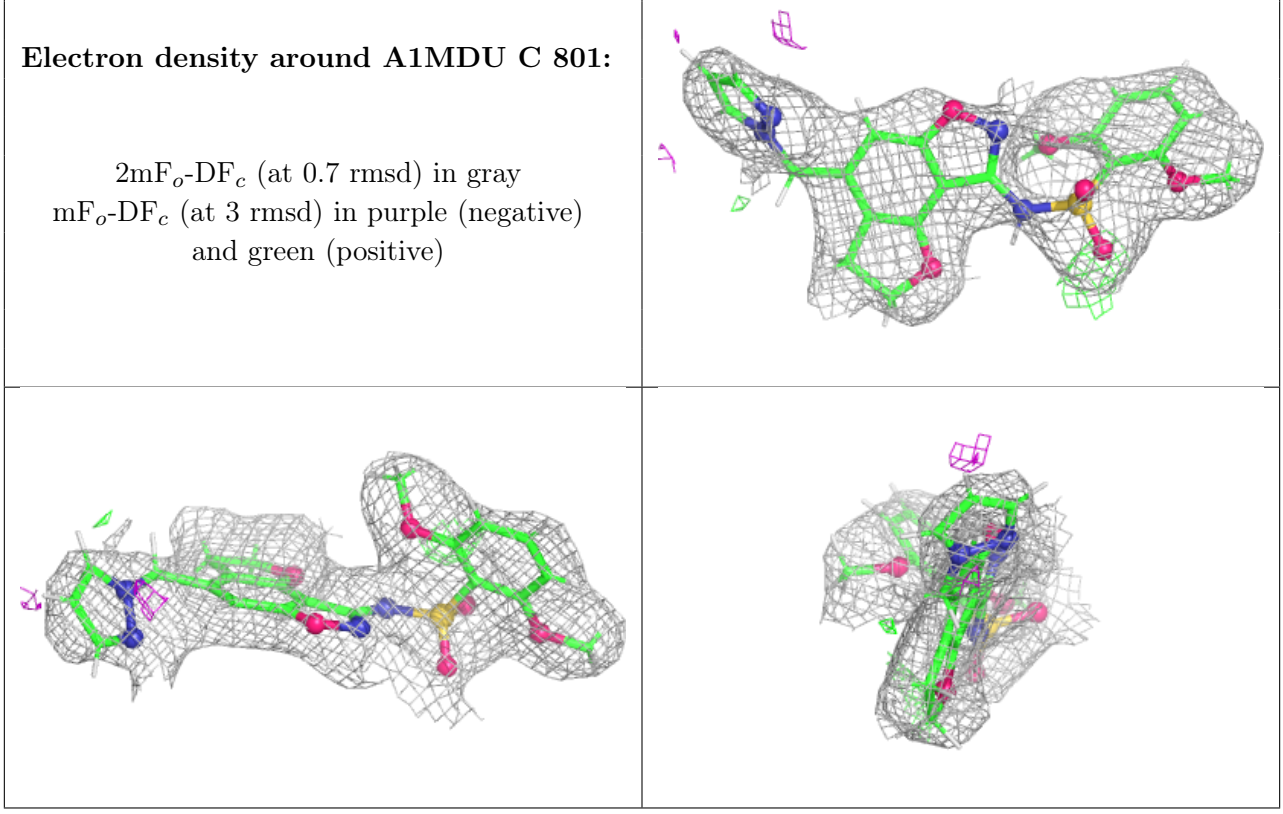






Electron density around A1MDU C 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.